

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032524\
 Data File : BM044752.D
 Acq On : 25 Mar 2024 12:51
 Operator : MA/JU
 Sample : PB159758BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 PB159758BL

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031324.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM044752.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.851	295	300	311	rVB	177571	277275	2.15%	0.398%
2	5.298	365	376	391	rBV	4928347	7229203	56.08%	10.387%
3	6.869	635	643	655	rBV	4462917	7250398	56.24%	10.418%
4	7.681	774	781	788	rBV	862107	1406522	10.91%	2.021%
5	8.851	969	980	988	rBV	2680082	4553596	35.32%	6.543%
6	10.463	1246	1254	1264	rBV	1113905	1886168	14.63%	2.710%
7	12.951	1669	1677	1690	rBV	5867079	8976981	69.64%	12.899%
8	14.333	1905	1912	1925	rVB	1518688	2291889	17.78%	3.293%
9	15.833	2159	2167	2181	rBV	4842323	7047132	54.67%	10.126%
10	17.086	2372	2380	2392	rBV	1907887	2744089	21.29%	3.943%
11	18.003	2529	2536	2551	rBV	1868106	2731434	21.19%	3.925%
12	19.286	2749	2754	2765	rBV	801848	1193235	9.26%	1.715%
13	19.439	2776	2780	2786	rVB2	263463	298655	2.32%	0.429%
14	19.733	2824	2830	2836	rBV	9958467	12891407	100.00%	18.523%
15	20.492	2955	2959	2965	rBV	215377	268215	2.08%	0.385%
16	21.286	3089	3094	3102	rBV	2455594	3121688	24.22%	4.485%
17	22.362	3274	3277	3282	rVB	205074	255020	1.98%	0.366%
18	22.874	3360	3364	3371	rVB	257449	393960	3.06%	0.566%
19	23.450	3458	3462	3468	rVB	353320	579965	4.50%	0.833%
20	23.527	3469	3475	3486	rVB	1505834	2978265	23.10%	4.279%
21	24.109	3569	3574	3583	rVB	342468	679651	5.27%	0.977%
22	24.868	3699	3703	3710	rVB	264476	541654	4.20%	0.778%

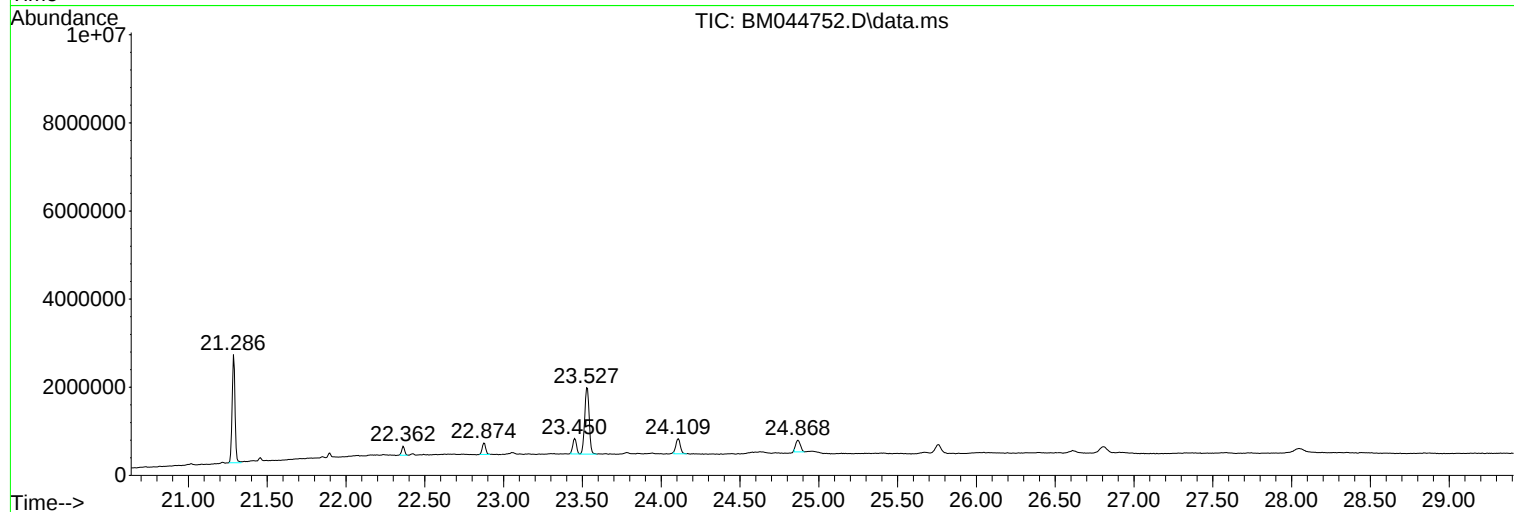
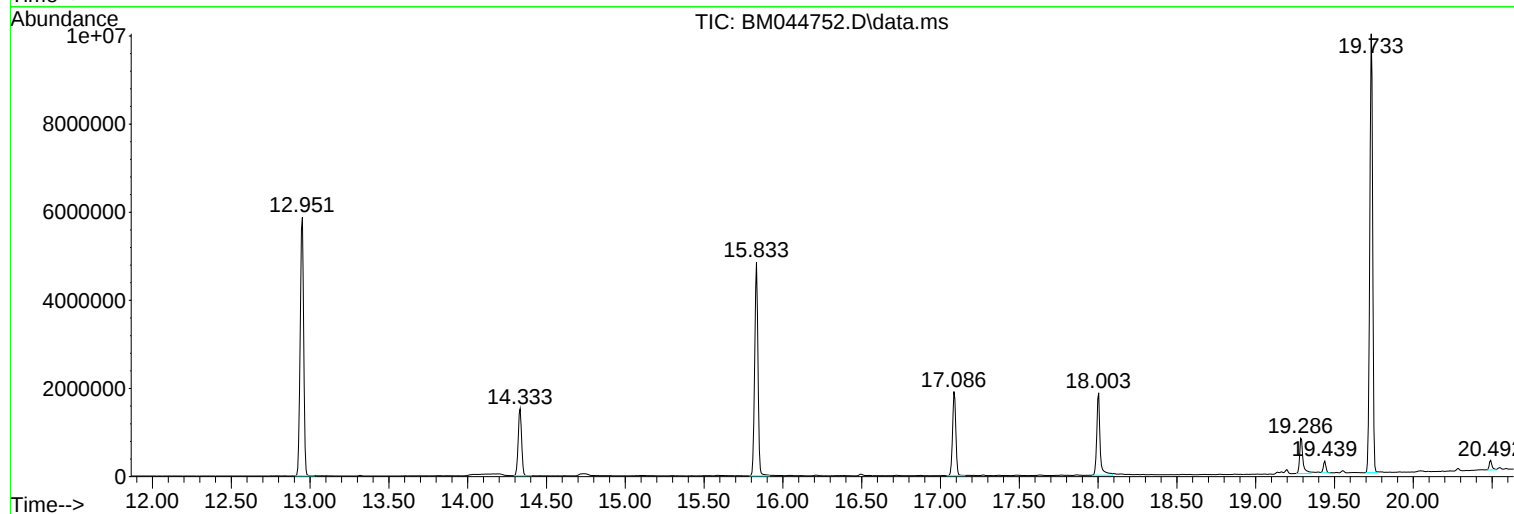
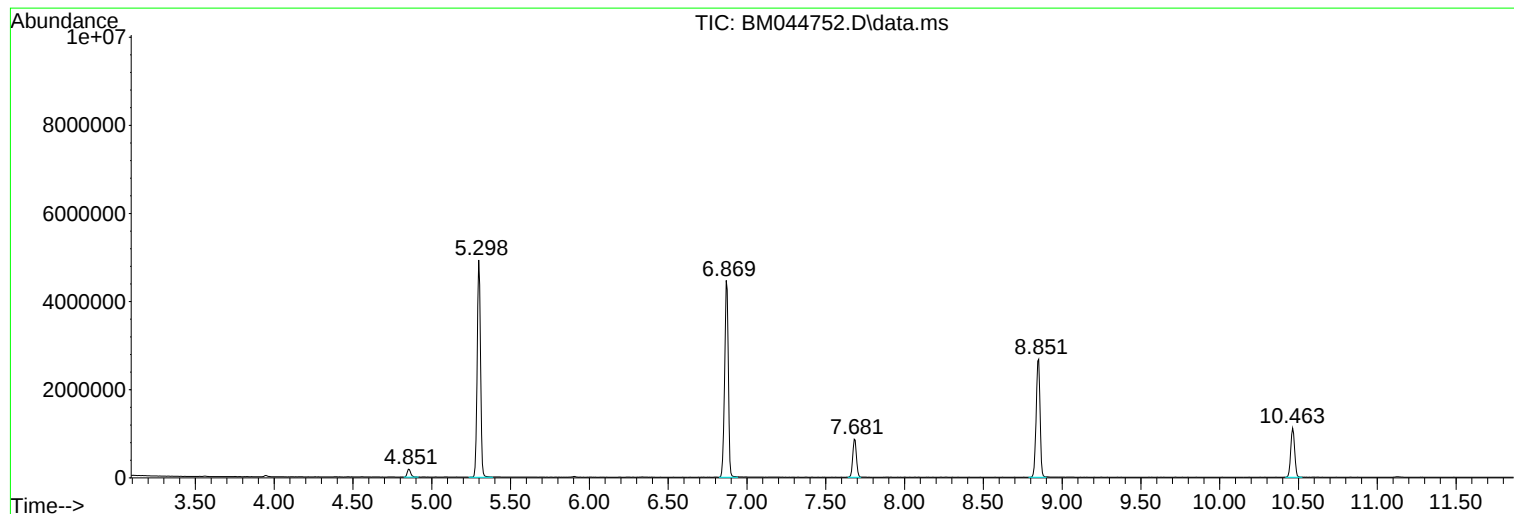
Sum of corrected areas: 69596402

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032524\
Data File : BM044752.D
Acq On : 25 Mar 2024 12:51
Operator : MA/JU
Sample : PB159758BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB159758BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032524\
Data File : BM044752.D
Acq On : 25 Mar 2024 12:51
Operator : MA/JU
Sample : PB159758BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB159758BL

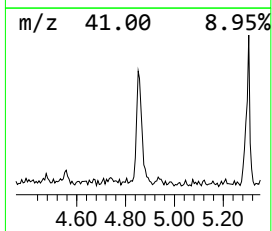
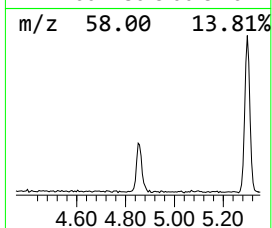
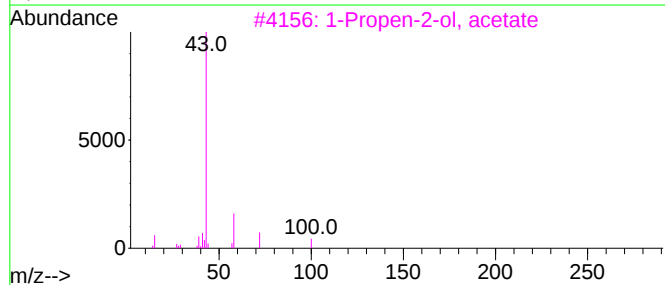
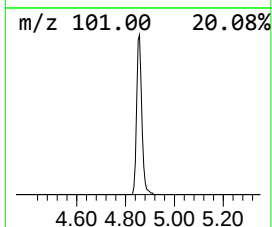
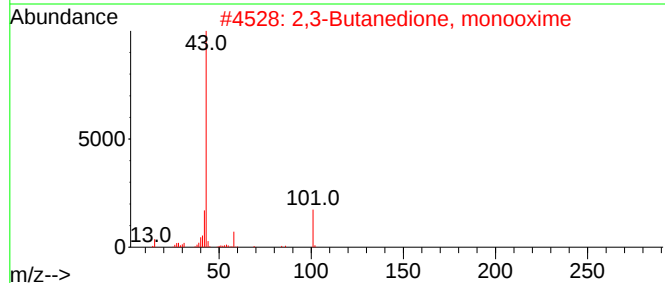
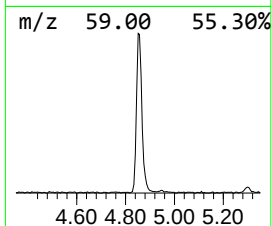
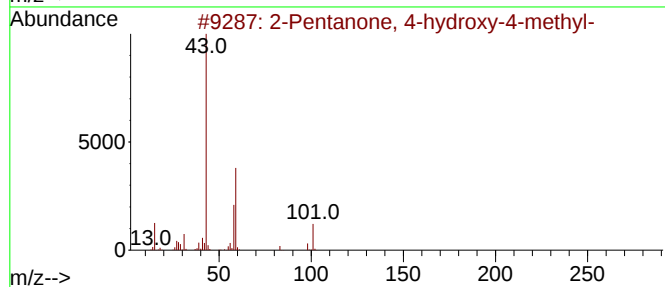
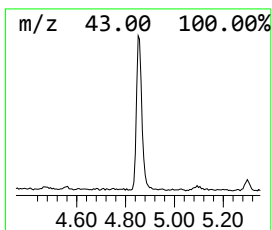
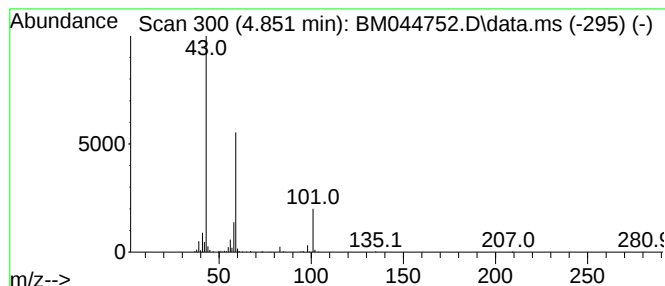
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.851	3.94 ng	277275	1,4-Dichlorobenzene-d4	7.686

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		Silane, dimethyl-	60	C2H8Si	001111-74-6	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032524\
Data File : BM044752.D
Acq On : 25 Mar 2024 12:51
Operator : MA/JU
Sample : PB159758BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB159758BL

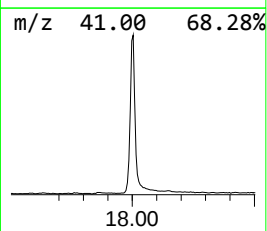
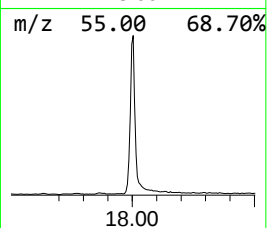
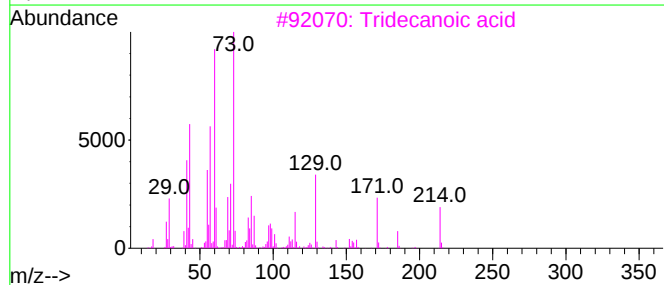
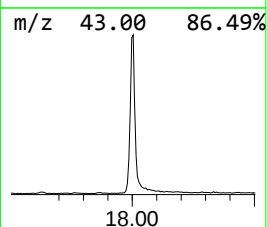
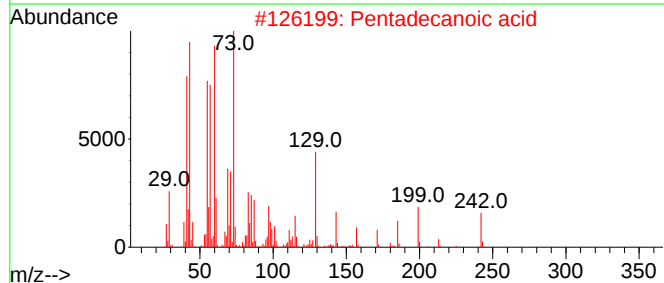
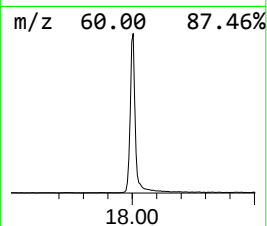
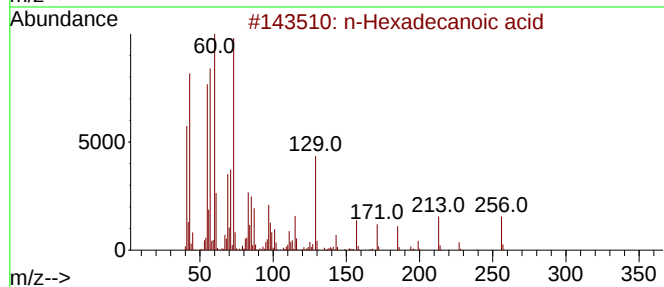
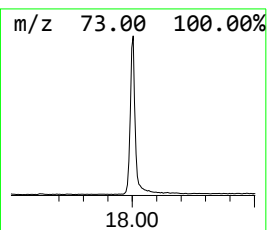
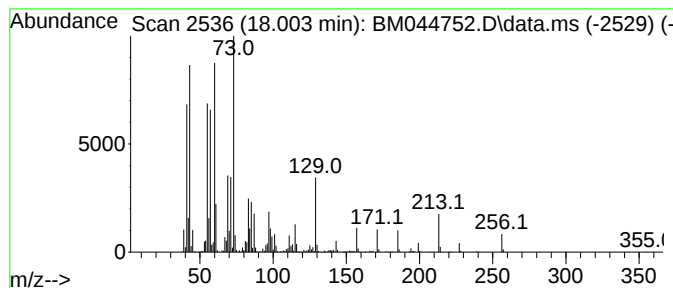
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.003	19.91 ng	2731430	Phenanthrene-d10	17.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			Tridecanoic acid	214	C13H26O2	000638-53-9	80
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5			Dodecanoic acid	200	C12H24O2	000143-07-7	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032524\
Data File : BM044752.D
Acq On : 25 Mar 2024 12:51
Operator : MA/JU
Sample : PB159758BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB159758BL

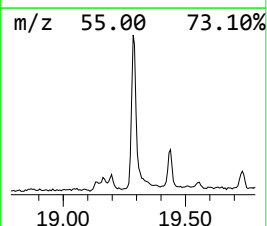
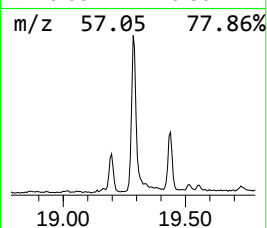
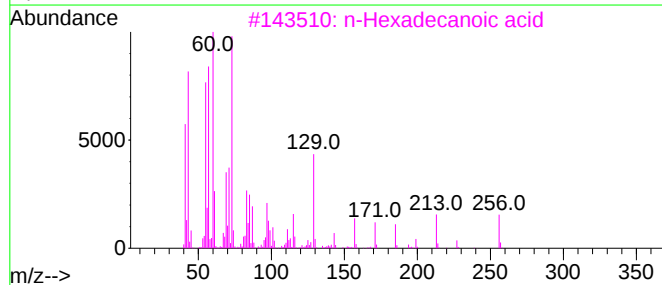
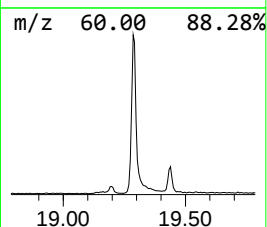
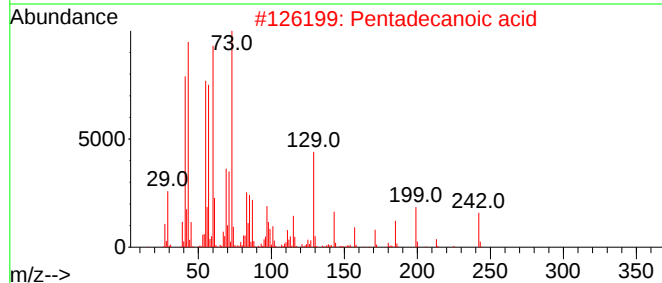
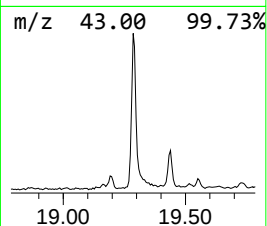
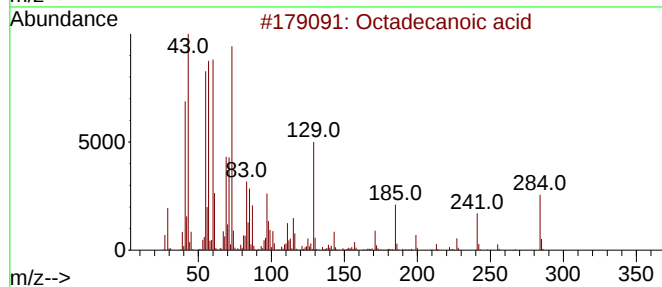
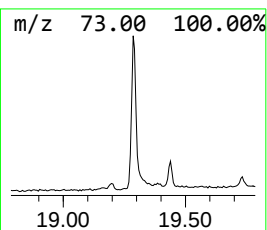
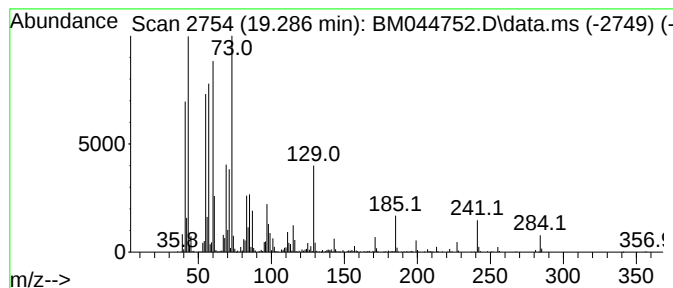
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.286	7.64 ng	1193240	Chrysene-d12	21.286

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	94
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5			n-Decanoic acid	172	C10H20O2	000334-48-5	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032524\
Data File : BM044752.D
Acq On : 25 Mar 2024 12:51
Operator : MA/JU
Sample : PB159758BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB159758BL

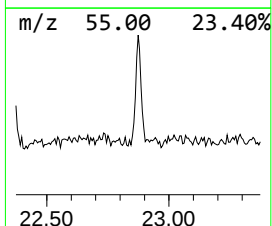
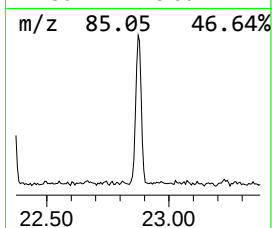
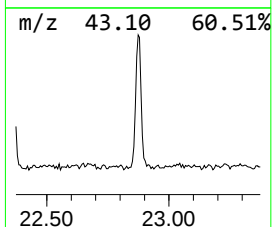
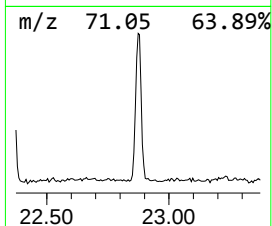
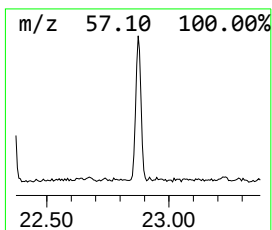
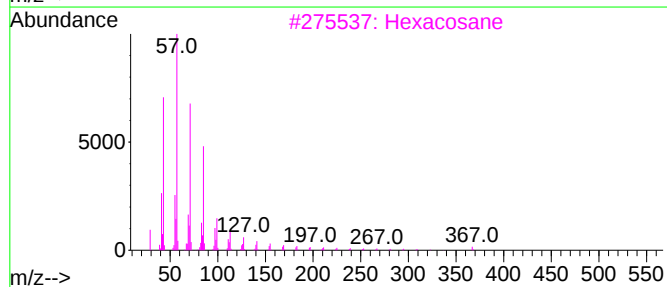
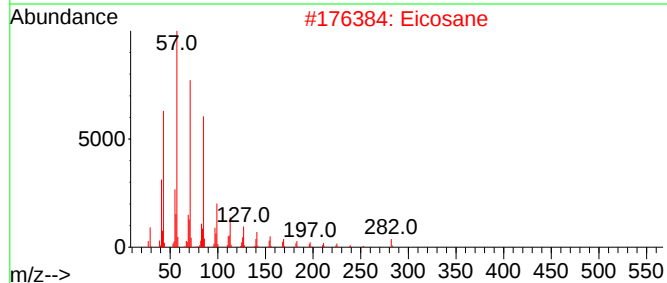
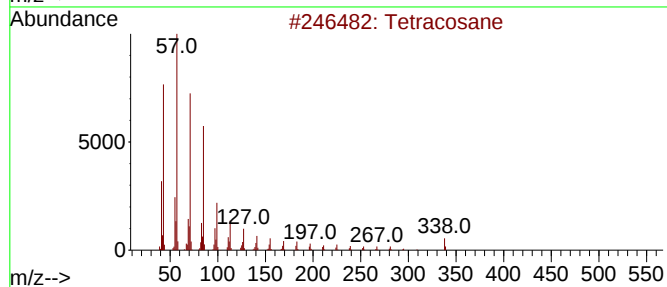
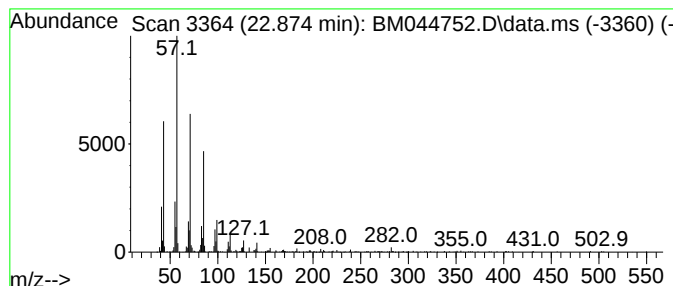
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Tetracosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.874	2.65 ng	393960	Perylene-d12	23.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	93
2			Eicosane	282	C20H42	000112-95-8	93
3			Hexacosane	366	C26H54	000630-01-3	90
4			Heptacosane	380	C27H56	000593-49-7	90
5			Octacosane	394	C28H58	000630-02-4	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032524\
Data File : BM044752.D
Acq On : 25 Mar 2024 12:51
Operator : MA/JU
Sample : PB159758BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB159758BL

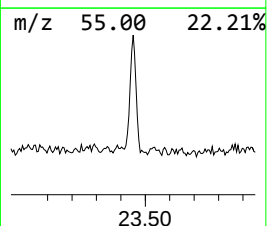
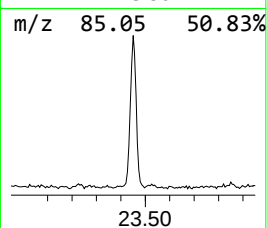
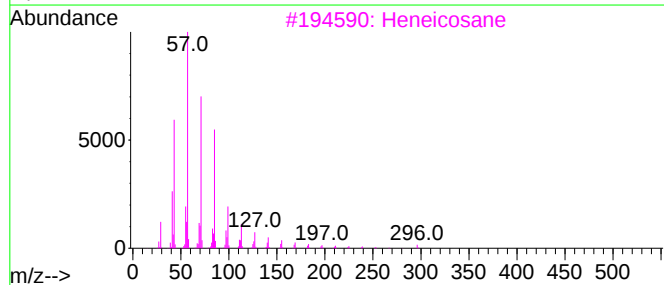
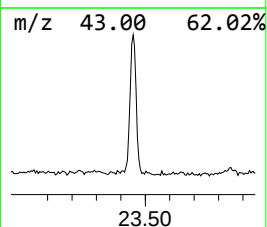
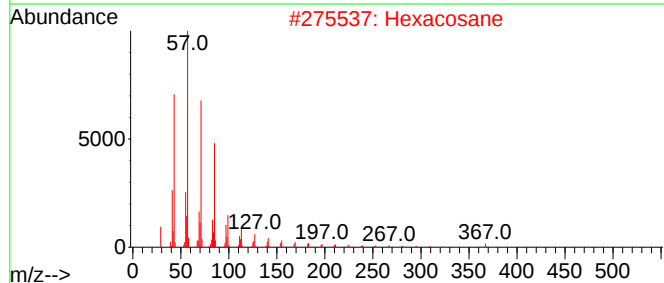
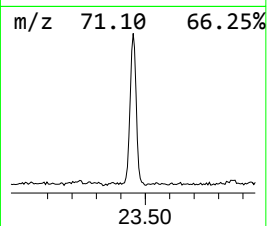
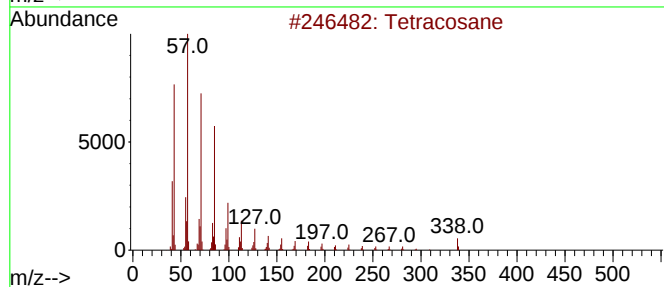
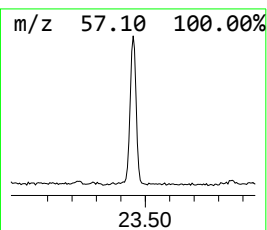
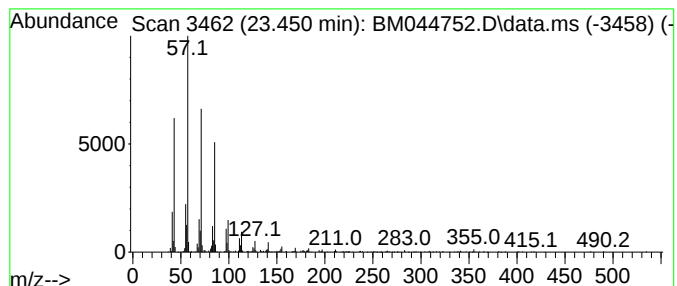
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.450	3.89 ng	579965	Perylene-d12	23.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	95
2			Hexacosane	366	C26H54	000630-01-3	90
3			Heneicosane	296	C21H44	000629-94-7	90
4			Disulfide, di-tert-dodecyl	402	C24H50S2	027458-90-8	83
5			Octadecane	254	C18H38	000593-45-3	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032524\
Data File : BM044752.D
Acq On : 25 Mar 2024 12:51
Operator : MA/JU
Sample : PB159758BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

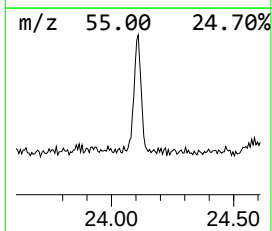
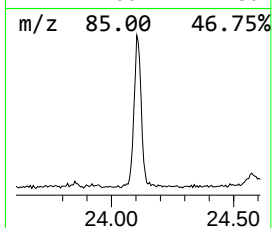
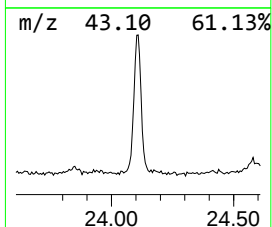
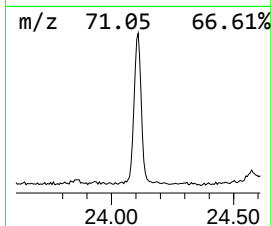
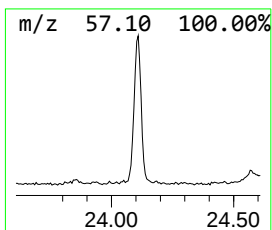
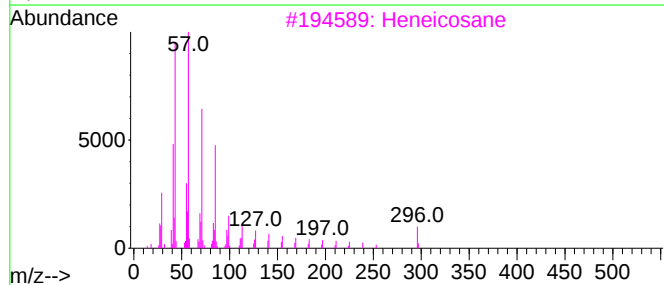
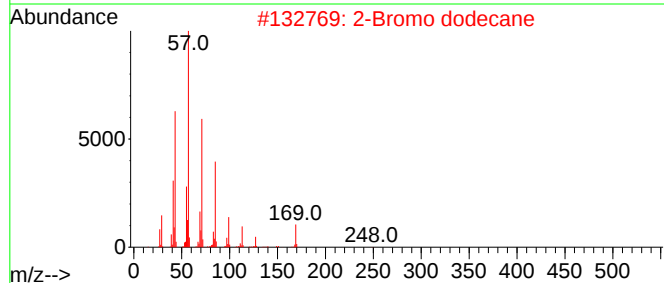
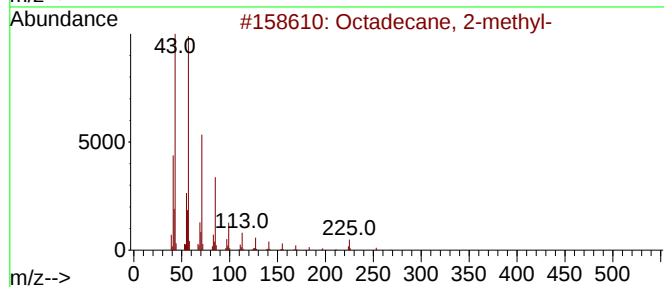
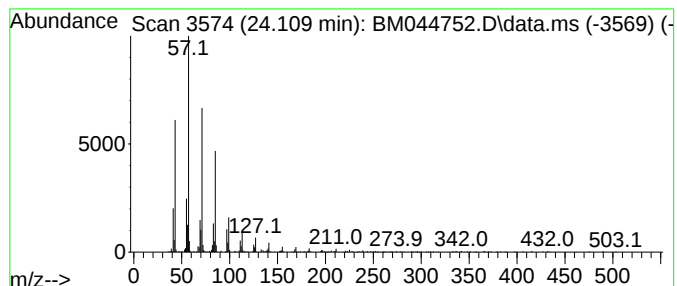
Instrument :
BNA_M
ClientSampleId :
PB159758BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Octadecane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
24.109	4.56 ng	679651	Perylene-d12	23.527	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 2-methyl-	268	C19H40	001560-88-9	93
2	2-Bromo dodecane	248	C12H25Br	013187-99-0	93
3	Heneicosane	296	C21H44	000629-94-7	91
4	Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
5	Hexacosane	366	C26H54	000630-01-3	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032524\
Data File : BM044752.D
Acq On : 25 Mar 2024 12:51
Operator : MA/JU
Sample : PB159758BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

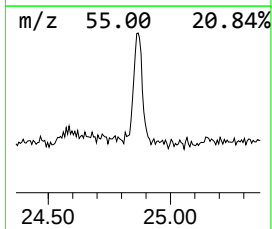
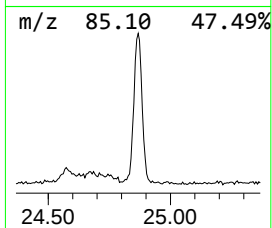
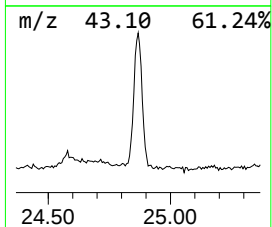
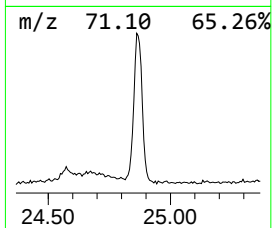
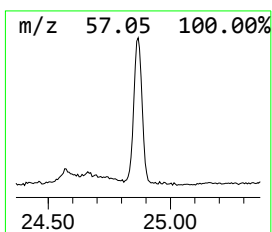
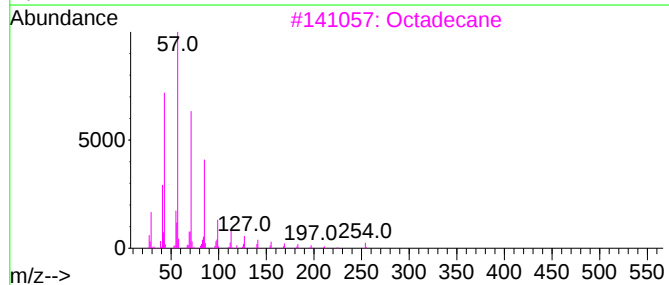
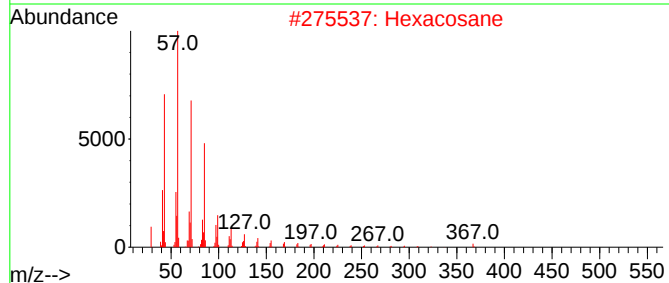
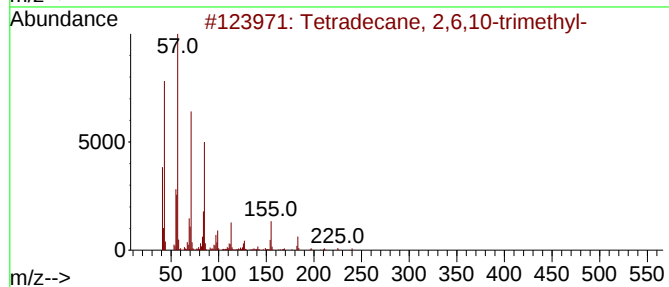
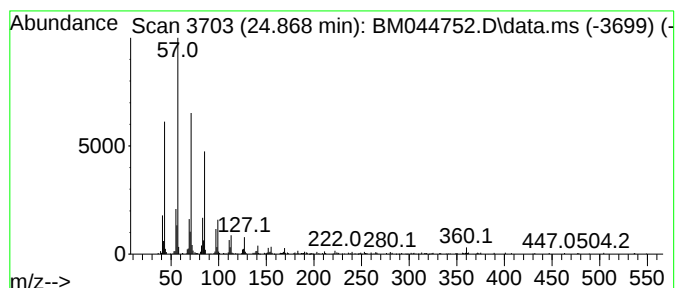
Instrument :
BNA_M
ClientSampleId :
PB159758BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Tetradecane, 2,6,10-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
24.868	3.64 ng	541654	Perylene-d12		23.527	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Tetradecane, 2,6,10-trimethyl-		240	C17H36	014905-56-7	90
2	Hexacosane		366	C26H54	000630-01-3	90
3	Octadecane		254	C18H38	000593-45-3	90
4	Eicosane, 10-methyl-		296	C21H44	054833-23-7	90
5	Octacosane, 2-methyl-		408	C29H60	001560-98-1	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032524\
Data File : BM044752.D
Acq On : 25 Mar 2024 12:51
Operator : MA/JU
Sample : PB159758BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB159758BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.851	3.9	ng	277275	1	7.686	1406520	20.0
n-Hexadecanoic ...	18.003	19.9	ng	2731430	4	17.086	2744090	20.0
Octadecanoic acid	19.286	7.6	ng	1193240	5	21.286	3121690	20.0
Tetracosane	22.874	2.6	ng	393960	6	23.527	2978270	20.0
Hexacosane	23.450	3.9	ng	579965	6	23.527	2978270	20.0
Octadecane, 2-m...	24.109	4.6	ng	679651	6	23.527	2978270	20.0
Tetradecane, 2,...	24.868	3.6	ng	541654	6	23.527	2978270	20.0